

2,5-Furandione  
108-31-6 | DTXSID7024166

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.01e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.22e-01

Confidence level: 5.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,3-Dioxolan-2-one</div> <div>Measured: 11.4</div> <div>Predicted: 4.54</div>	<div>Image not found</div> <div>6-Methyl-2H-pyran-2,4(3H)-dione</div> <div>Measured: 7.61e-02</div> <div>Predicted: 2.49e-01</div>	<div>Image not found</div> <div>Propylene carbonate</div> <div>Measured: 1.71</div> <div>Predicted: 1.93</div>
<div>Image not found</div> <div>3-Acetyldihydro-2(3H)-furanone</div> <div>Measured: 1.56</div> <div>Predicted: 8.04e-01</div>	<div>Image not found</div> <div>Protoanemonin</div> <div>Measured: 1.04e-01</div> <div>Predicted: 2.33e-01</div>	